

# Effective-interaction approach to the many-boson problem

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We show that the convergence behavior of the many-body numerical diagonalization scheme for strongly interacting bosons in a trap can be significantly improved by the Lee-Suzuki method adapted from nuclear physics: One can construct an effective interaction that acts in a space much smaller than the original Hilbert space. In particular for short-ranged forces and strong correlations, the method offers a good estimate of the energy *and* the excitation spectrum, at a computational cost several orders of magnitude smaller than that required by the standard method.

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The many-body problem of interacting bosons or fermions poses a continuous challenge for quantum physics. The complexity of the quantum states increases quickly with higher particle numbers or stronger correlations, making it essentially impossible to solve the many-body problem exactly. Thus, mean-field methods are often applied, being numerically much less demanding than any attempt to diagonalize the many-body Hamiltonian. Examples are the Gross-Pitaevskii approach for trapped bosons [1, 2, 3], or the celebrated Kohn-Sham equations [4, 5] for fermions, as often used in the local (spin) density approximation. However, these methods can treat correlations only in an approximate way, and are proven insufficient for strong interactions between the particles. Quantum Monte Carlo calculations provide an alternative approach in many cases (see for example, the review by Harju [6]), but have other drawbacks, such as limited accessibility of the excitation spectrum, a problem shared by the other methods. The development of alternative diagonalization methods such as, e.g., coupled cluster methods [7] is an urgent issue.

Facing the above problems with strong interactions, one quickly realizes that often, the only method of choice is the straightforward numerical diagonalization of the many-body Hamiltonian. In fact, this has been tried for a large variety of physical problems, ranging from nuclear structure (see for example, the review by Caurier *et al.* [8]) and quantum chemistry to artificially made quantum systems such as metallic clusters [9] and quantum dots [10]. However, with increasing particle number or stronger interactions between the particles, the number of basis states needed for an accurate description of the many-body quantum system increases beyond computational reach. Truncations of Hilbert space become necessary – but often, for the reduced basis, the results are too inaccurate [11].

In nuclear physics, a significant step forward has been achieved by applying the Lee-Suzuki method [12, 13], that prescribes unitary transformations on operators (e.g. the Hamiltonian) to obtain effective operators within the reduced basis space. This method has been successfully used in so called no-core shell model calculations, for example, where nuclear systems with  $\sim 12$  fermions have

been studied [14].

Since the experimental realization of Bose-Einstein condensation with cold, trapped atoms, much interest turned to the physics of harmonically confined many-boson systems. Although the trapping potentials today confine thousands of bosons, the few-body regime does not seem to be impossible to reach, having in mind also the recent advances with optical lattices [15]. Increasing technological expertise with Bose-Einstein condensates “on chips” [16], together with the newly emerging research area of “atomtronics” [17], makes the need for further theoretical developments for a description of cold-atom gases with strong correlations an urgent issue.

In this Letter, we apply the Lee-Suzuki method – to the best of our knowledge, for the first time – to a system of harmonically trapped spinless *bosons* with short-ranged repulsive interactions. The fact that the Lee-Suzuki method works very well for the strong short-ranged interactions between the nucleons encourages its application to describe cold atom gases beyond mean-field.

At this point we note that there exist alternative ways of doing the unitary transformation. Two examples, so called renormalization group transformations, are “ $V_{low-k}$ ” [18] and SRG (similarity renormalization group) [19]. SRG is frequently used in nuclear physics [20]. Another example, related to SRG, is UCOM (unitary correlation operator method) [21]. In future studies, it would be interesting to try alternative methods for the problem at hand, but here we have focused on the Lee-Suzuki transformation. Another study which applies the Lee-Suzuki transformation on a non-nuclear system is [22], in which the two-electron problem in a quantum dot is examined. Also, in [23, 24] the few-body problem of a trapped Fermi gas is investigated with techniques similar to what is used here.

For an ultra-cold gas of neutral atoms, the interaction between the particles can often be modeled by a short-range potential. We choose to use a Gaussian distribution function parameterized by a range  $\sigma$ , and a strength coefficient  $g$ . We here let the system be (quasi-) two-dimensional. The Hamiltonian is

Interaction strength $g$	Range $\sigma$	Scattering length $a$
1	0.1	0.000283
10	0.1	0.0871
10	1	0.871

Table I: Numerically calculated s-wave scattering lengths for some parameter choices of the interaction potential (all quantities in oscillator units).

$$\hat{H} = \sum_{i=1}^N \frac{\hat{\mathbf{p}}_i^2}{2m} + \frac{1}{2}m\omega^2\mathbf{r}_i^2 + \frac{1}{2}\sum_{j \neq i}^N g \frac{1}{2\pi\sigma^2} \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_j|^2}{2\sigma^2}\right),$$

where  $N$  is the number of particles and  $m$  is the particle mass. The chosen interaction is normalized so that it becomes a  $\delta$ -function in the limit when  $\sigma$  goes to zero, which also allows us to avoid the mathematical difficulties of point-interactions in connection to the diagonalization of the full many-body Hamiltonian [25]. In a cold atomic gas, the strength coefficient  $g$  is related to the scattering length between the particles. The scattering length can in some systems be experimentally tunable by Feshbach resonances [3]. The typical length scale of the system is the oscillator length,  $\sqrt{\hbar/(m\omega)}$ . The range of the interaction in ultra-cold atomic gases is typically very short compared to the wavelength of the particles; here we pick  $\sigma = 0.1\sqrt{\hbar/(m\omega)}$  for our calculations (in the following the oscillator length unit is used). This parameter will be discussed in more detail later.

In two dimensions, the (s-wave) scattering length,  $a$ , is usually defined to be a positive quantity, see for example Ref. [26]. A two-body system will have at least one bound state when the scattering length is larger than the distance outside which the interaction potential is zero. However, a purely repulsive short-range potential produces a scattering length that is smaller than the range of the potential. For such systems, an increased attraction (or reduced repulsion) would decrease  $a$  towards zero and an even stronger attraction would produce a bound state and give an  $a$  decreasing from infinity. The scattering lengths corresponding to the repulsive interaction potential used here can be calculated numerically, see table I.

The short-range interaction between the particles induces short-range correlations, thus one would need a very large set of basis states in order to accurately describe the wavefunction and to obtain a good estimate of the energy of the system. However, one may perform a unitary transformation of the Hamiltonian so that states within a given model space become decoupled from the ones in the complementary excluded space [12, 13]. The finite model space and the complementary infinite space can be defined by the projection operators  $\hat{P}$  and  $\hat{Q}$ , respectively. The original Hamiltonian of the system is transformed to an effective Hamiltonian acting only in a subspace of the complete Hilbert space, while preserving

a subset of the original eigenvalues. Thus, given the effective Hamiltonian, the computational effort in finding the eigenvalues can be reduced. However, even though the original Hamiltonian contains only one- and two-body terms, the effective Hamiltonian will in general be an  $N$ -body operator. So far, no approximation has been introduced, only an operator transformation given by:

$$\hat{H}_{\text{eff}} = \frac{\hat{P} + \hat{P}\hat{\xi}^\dagger\hat{Q}}{\sqrt{\hat{P} + \hat{\xi}^\dagger\hat{\xi}}} \hat{H}_{\text{original}} \frac{\hat{Q}\hat{\xi}\hat{P} + \hat{P}}{\sqrt{\hat{P} + \hat{\xi}^\dagger\hat{\xi}}}, \quad (1)$$

where  $\hat{\xi}$  is an operator acting as a mapping between the  $P$ - and  $Q$ -spaces, satisfying  $\hat{\xi} = \hat{Q}\hat{\xi}\hat{P}$ . Note that the transformation (1) is unitary and yields an effective Hamiltonian that is energy-independent and hermitian.  $\hat{H}_{\text{eff}}$  does not couple states in the  $P$ -space with states in the  $Q$ -space.

Unfortunately, to find the mapping operator  $\hat{\xi}$  one needs the exact solution of the  $N$ -body problem, which is in itself the final goal. Our simplest, yet nontrivial, approximation is to develop a two-body effective Hamiltonian. The approximation consists in finding  $\hat{\xi}_2$  for the two-body problem and to compute an effective Hamiltonian for the two-body system. By subtracting the one-body terms (kinetic + potential energy) one thus obtains an effective two-body interaction. This effective interaction is then used to construct the  $N$ -body effective Hamiltonian that will now contain only one- and two-body terms. Due to the approximation of the effective Hamiltonian, the obtained energies will not be bound by the variational theorem. This particular property of the current method is in contrast to the situation encountered when using standard configuration interaction calculations, or quantum Monte-Carlo approaches.

Although this approach can lead to good estimates of the energy eigenvalues, the obtained eigenvectors are incorrect since they do not contain components from the excluded  $Q$ -space. However, the eigenvectors are often not interesting by themselves; only observables, expressed as expectation values of physical operators, are relevant. Transformations similar to the one performed on the Hamiltonian, can be applied to other operators so that their expectation values can be obtained from the  $P$ -space eigenvectors. In the present study, however, we restrict the discussion to the many-body energy spectrum.

For bosons, the many-body basis states are permanents, with  $N$  particles distributed over the single-particle orbitals of the system. The truncation of the infinite basis is performed in the following way: Neglecting interactions, the state of lowest energy is the one with all  $N$  bosons in the lowest orbital as defined by the confinement potential, with energy  $E = \hbar\omega N$ . We incorporate in the  $P$ -space all many-body states with an energy

$$E \leq \hbar\omega(N + \mathcal{N}_{\text{max}}),$$

so that  $\mathcal{N}_{\max}$  is a parameter determining the maximum allowed energy of particle-hole excitations from the state of lowest energy. The number of included states increases rapidly with  $\mathcal{N}_{\max}$ .

In addition, all possible combinations of two particles found in the  $N$ -body model space ( $P$ ) defines the restricted space of the two-body system ( $P_2$ ) that is used to compute the effective interaction. Having defined  $P_2$ , the Hamiltonian for the complete two-body space is transformed. In practice, the complete two-body space must of course also be truncated. To this aim we take all two-body states that can be constructed using the first 20 harmonic oscillator shells.

The original Hamiltonian preserves angular momentum ( $L$ ), implying that we can restrict the basis to states with a given value of  $L$ , thus limiting its size. We confirm that the effective interaction also preserves angular momentum (within numerical accuracy).

First we use the method to calculate energies of a system with only four particles,  $N = 4$ , with an interaction range  $\sigma = 0.1$ . Here, we consider only states with zero angular momentum. For such a small system, the standard configuration interaction method can be applied. Figure 1 shows results from both types of calculations. For  $g = 1$ , both methods give good energy estimates already at small  $\mathcal{N}_{\max}$ . But for  $g = 10$  the standard calculations require a large basis set to obtain a reasonably converged energy estimate, while the effective interaction provides an answer with significantly less computational effort. Typically, for an  $\mathcal{N}_{\max}$  around 5, the basis size is of order 10, while for  $\mathcal{N}_{\max}$  around 25 it is of order  $10^4$ . These numbers depend strongly on the system parameters  $N$  and  $L$ , though.

Note that for  $\mathcal{N}_{\max} = 0$ , the standard configuration interaction calculation reduces to a perturbative calculation, where the energy grows linearly with the strength of the interaction,  $g$ . In addition, for sufficiently large  $\mathcal{N}_{\max}$  the two methods will be equivalent, since the  $P$ -space is then actually the full space.

The method works well both for the ground state energy and the excitations. An interesting observation is that for  $g = 10$ , at  $\mathcal{N}_{\max} = 6$  the standard calculation shows a degeneracy in the first excited state. This effect is spurious, however, since the energies split up when a larger basis is used. When using the effective interaction, this false degeneracy does not occur.

Let us now turn to systems with larger number of particles. Figure 2 shows calculations for  $N = 9$  bosons. In the case of  $g = 1$  the effective interaction method again very rapidly produces an accurate estimate of the energy. For  $g = 10$ , where the correlations in the systems are much stronger than for  $g = 1$ , the energies obtained when using effective interactions appear to have reached some plateau, but still show a slow decrease with growing  $\mathcal{N}_{\max}$ . In comparison, the energies obtained from the standard calculations show a much slower convergence.

The convergence behavior for an even larger system of  $N = 20$  particles is shown in Fig. 3. In the case of  $g = 1$

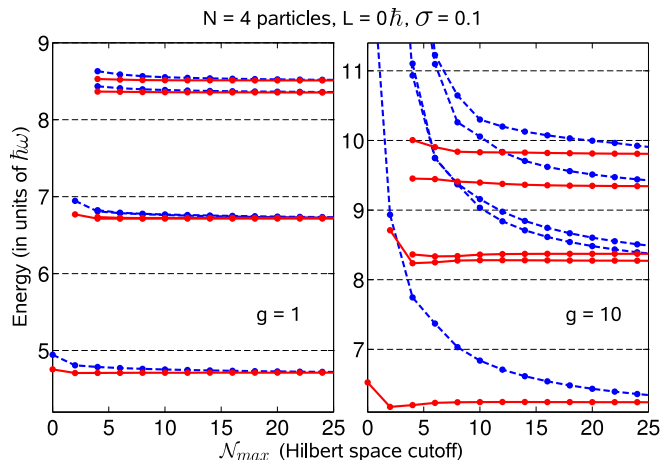


Figure 1: Energies for a system of  $N = 4$  bosons and total angular momentum  $L = 0\hbar$ , for different cutoffs of the many-body Hilbert space (parameterized by  $\mathcal{N}_{\max}$ ). The range of the interaction is  $\sigma = 0.1$ , and two different strengths ( $g$ ) are shown. The *blue dashed* curves are the results from standard configuration interaction calculations, while the *red solid* curves are energies obtained using the effective interaction approach. While the standard calculations require a large basis set to give a good energy estimate, the effective interaction provides roughly the same answer with significantly less computational effort. (Please note that for small  $\mathcal{N}_{\max}$ , there are very few states in the  $P$ -space, and consequently only a few eigenvalues can be obtained.)

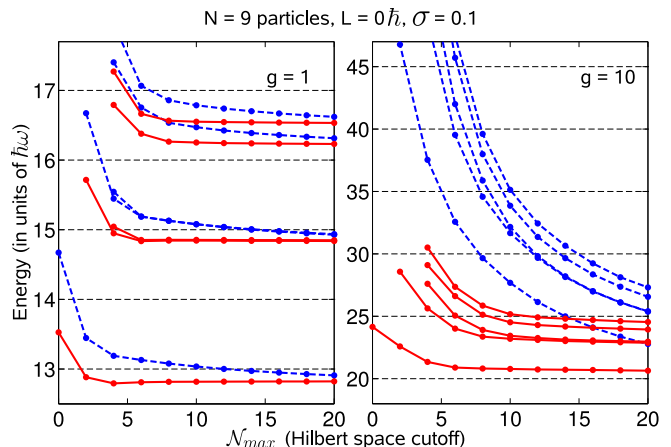


Figure 2: Same as Fig. 1 but for  $N = 9$  bosons. Note the rapid convergence of energies using the effective interaction approach. For example, we note that in this case a calculation with  $\mathcal{N}_{\max} = 6$  requires 12 basis states, while  $\mathcal{N}_{\max} = 20$  would correspond to 81097 states.

it is possible to reach fairly converged results with both methods. When  $g = 10$  neither method is able to provide converged energies for the range of  $\mathcal{N}_{\max}$  considered here. An intuitive interpretation would be that  $\mathcal{N}_{\max}$  should be of the same order as  $N$ , allowing about one extra unit of energy per particle, so that every particle has some freedom to adjust in the system. Since the number of

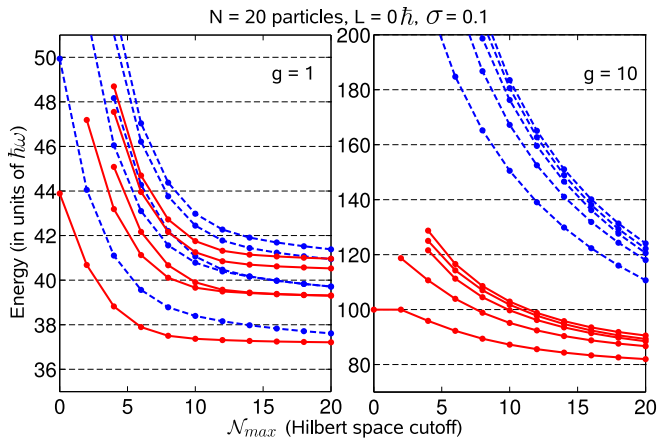


Figure 3: Same as Fig 1 but for  $N = 20$  bosons. For  $g = 10$ , the energy obtained using effective interaction cannot be said to be converged as a function of  $N_{\max}$ .

basis states grows very rapidly with both  $N$  and  $N_{\max}$ , it seems that the method is most suitable in the strongly correlated regime; and makes it possible to study larger, but not much larger, systems than with the standard method.

All results shown so far involved the  $L = 0\hbar$  (non-rotating) states of the different systems studied. However, the method is not restricted to the non-rotating case. Figure 4(a) shows the energies for a system of  $N = 9$  bosons, at angular momentum  $L = 9\hbar$ . Here, the energy is not a strictly decreasing function of  $N_{\max}$ , but aside from this the convergence is similar to that seen in figure 2. An energy obtained with the standard configuration interaction method is always an upper bound to the true value, since it is a variational approach. As the size of the basis space is increased, a better or equally good estimate is found. Calculations using an approximated effective Hamiltonian, as in this study, are not variational so higher-order terms may contribute with either sign to the energy.

The Lee-Suzuki approach was invented to handle the short-range correlations in nuclei [12, 13], and the short range of the interaction is known to be essential for the performance of the method. For all results presented this far, we have set the range parameter  $\sigma = 0.1$ . Figure 4(b) shows results with a larger range,  $\sigma = 1$ , for a system with  $N = 9$  particles. Apart from some deviations for small  $N_{\max}$ , the effective interaction here does not give an improved convergence rate compared to the standard calculations. This result suggests that for  $\sigma$  smaller than 0.1 the method would perform even better than demonstrated in e.g. figure 2. However, the numerical solution of the two-body problem becomes more difficult with decreasing  $\sigma$ , and our present implementation prevents us from exploring smaller  $\sigma$ .

As mentioned, the correct effective Hamiltonian would

in general be an  $N$ -body operator. It would be interesting to examine how inclusion of e.g. an effective three-body

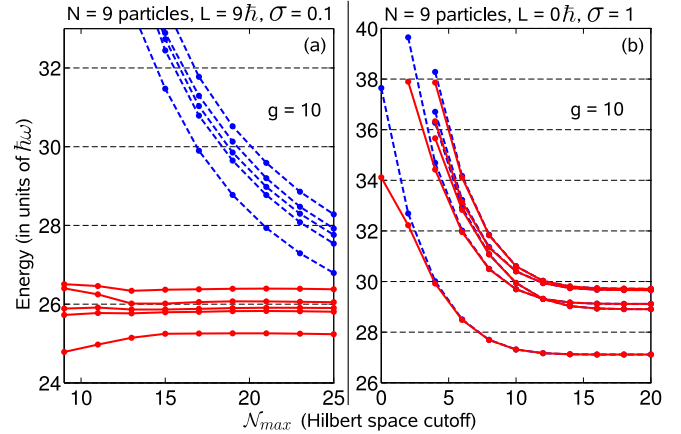


Figure 4: (a) Energy levels (in units of  $\hbar\omega$ ) for a system of  $N = 9$  bosons and angular momentum  $L = 9\hbar$  (in this case there are no possible basis states for  $N_{\max} < 9$ ). (b) Energies for a system with  $N = 9$  and interaction range  $\sigma = 1$  ( $L = 0\hbar$  states). See caption of figure 1 for explanations.

interaction would affect the numerical convergence, although the two-body approximation is exact in the limit  $N_{\max} \rightarrow \infty$ . As seen in our results, the obtained energies typically converge rapidly as functions of  $N_{\max}$ , implying that an effective two-body Hamiltonian is sufficient in many situations.

To summarize, in order to calculate properties of cold, bosonic atomic gases with strong short-range interactions between the particles, we have employed a unitary transformation of the Hamiltonian. The transformation is used to recover correlation effects which would otherwise be lost within the heavily truncated basis space we consider. The method is in practice a modification of the standard configuration interaction approach. In many cases it produces a good estimate of the energy, with a computational effort which is several orders of magnitude smaller than that required by the standard method. The main advantage, compared to many other approaches, is the accessibility of the excitation spectrum with *significantly* reduced numerical effort.

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- [1] E.P. Gross, *Nuovo Cimento* **20**, 454 (1961); L.P. Pitaevskii, *Zh. Eksp. Teor. Fiz.* **40**, 646 (1961) [*Sov. Phys. JETP* **13**, 451 (1961)]
  - [2] A.J. Leggett, *Rev. Mod. Phys.* **73**, 307 (2001)
  - [3] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation*, Oxford University Press, Oxford (2003)
  - [4] W. Kohn and L.J. Sham, *Phys. Rev.* **140**, A1133 (1965)
  - [5] W. Kohn, *Rev. Mod. Phys.* **71**, 1253 (1999)
  - [6] A. Harju, *J. Low Temp. Phys.* **140**, 181 (2005)
  - [7] L.S. Cederbaum, O.E. Alon and A.I. Streltsov, *Phys. Rev. A* **73**, 043609 (2006)
  - [8] E. Caurier, *et al.*, *Rev. Mod. Phys.* **77**, 427 (2005)
  - [9] M. Koskinen, M. Manninen and P.O. Lipas, *Phys. Rev. B* **49**, 8418 (1994)
  - [10] S.M. Reimann and M. Manninen, *Rev. Mod. Phys.* **74**, 1283 (2002)
  - [11] O.E. Alon, A.I. Streltsov, K. Sakmann and L.S. Cederbaum, *Europhys. Lett.* **67**, 8 (2004)
  - [12] K. Suzuki and S.Y. Lee, *Prog. Theor. Phys.* **64**, 2091 (1980); K. Suzuki, *Prog. Theor. Phys.* **68**, 246 (1982); K. Suzuki and R. Okamoto, *Prog. Theor. Phys.* **70**, 439 (1983)
  - [13] K. Suzuki, *Prog. Theor. Phys.* **68**, 1999 (1982); K. Suzuki and R. Okamoto, *Prog. Theor. Phys.* **92**, 1045 (1994)
  - [14] P. Navratil, J.P. Vary and B.R. Barrett, *Phys. Rev. Lett.* **84** 5728 (2000); P. Navratil, J.P. Vary and B.R. Barrett, *Phys. Rev. C* **62** 054311 (2000)
  - [15] O. Morsch and M. Oberthaler, *Rev. Mod. Phys.* **78**, 179 (2006)
  - [16] R. Folman, P. Kruger, D. Cassettari, B. Hessmo, T. Maier and J. Schmiedmayer, *Phys. Rev. Lett.* **84**, 4749 (2000)
  - [17] B. T. Seaman, M. Kramer, D.Z. Anderson and M.J. Holland, *Phys. Rev. A* **75**, 023615 (2007)
  - [18] S K Bogner, T T S Kuo and A Schwenk, *Phys. Rep.* 386, 1-27 (2003)
  - [19] S D Glazek and K G Wilson, *Phys. Rev. D* **48**, 5863 (1993). F. Wegner, *Annalen der Physik (Leipzig)* 3, 77 (1994)
  - [20] S K Bogner, R J Furnstahl and R J Perry, *Phys. Rev. C* **75**, 061001(R) (2007)
  - [21] H Hergert and R Roth, *Phys. Rev. C* **75**, 051001(R) (2007)
  - [22] S. Kvaal, M. Hjorth-Jensen and Halvor Moell Nilsen, *Phys. Rev. B* **76**, 085421 (2007)
  - [23] I. Stetcu, B.R. Barrett, U. van Kolck and J.P. Vary, *Phys. Rev. A* **76**, 063613 (2007)
  - [24] Y. Alhassid, G.F. Bertsch and L. Fang, *Phys. Rev. Lett.* **100**, 230401 (2008)
  - [25] K. Huang, *Statistical Mechanics*, John Wiley & Sons, New York (1987)
  - [26] B J Verhaar, J P H W van den Eijnde, M A J Voermans and M M J Schaffrath, *J. Phys. A: Math. Gen.* **17** 595-598 (1984)